```
=> d his

     (FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

     FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3             24 S L1 SSS FULL
L4              0 S L2 SSS
L5              3 S L2 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004
L6             11 S L3
L7              2 S L3 AND L5
L8              7 S L3/PREP
L9              2 S L8 AND L5
L10             2 S L7 OR L9

     FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004
L11               STRUCTURE UPLOADED
L12             0 S L11

=> d l11
L11 HAS NO ANSWERS
L11               STR
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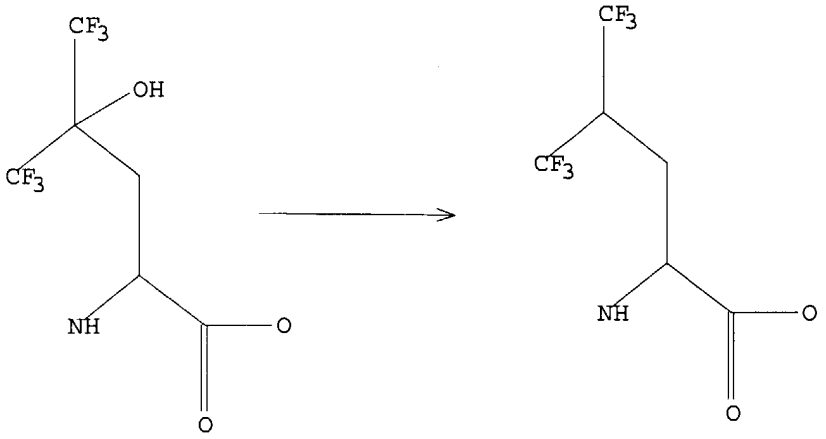


```
Structure attributes must be viewed using STN Express query preparation.


=> s l11
SAMPLE SEARCH INITIATED 11:18:24 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM      0 DOCUMENTS

100.0% DONE      0 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:          0 TO         0
PROJECTED ANSWERS:                0 TO         0

L13             0 SEA SSS SAM L11 (      0 REACTIONS)

=>
```

```
=> d his

     (FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

     FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3             24 S L1 SSS FULL
L4              0 S L2 SSS
L5              3 S L2 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004
L6             11 S L3
L7              2 S L3 AND L5
L8              7 S L3/PREP
L9              2 S L8 AND L5
L10             2 S L7 OR L9

     FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004
L11               STRUCTURE UPLOADED
L12             0 S L11
L13             0 S L11

     FILE 'CAPLUS' ENTERED AT 11:20:56 ON 20 APR 2004

     FILE 'REGISTRY' ENTERED AT 11:38:23 ON 20 APR 2004
L14               STRUCTURE UPLOADED
L15             2 S L14

     FILE 'CAPLUS' ENTERED AT 11:38:42 ON 20 APR 2004
L16             3 S L15
L17             0 S L16 AND L7
L18             0 S L16 AND L6
L19             0 S L5 AND L15

=> d l15
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n


=> d l14
L14 HAS NO ANSWERS
L14                STR
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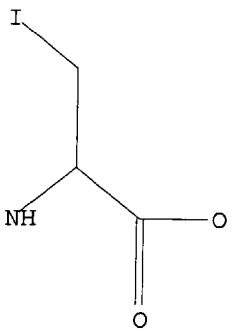


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Structure attributes must be viewed using STN Express query preparation.

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=> d his

     (FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

     FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3             24 S L1 SSS FULL
L4              0 S L2 SSS
L5              3 S L2 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004
L6             11 S L3
L7              2 S L3 AND L5
L8              7 S L3/PREP
L9              2 S L8 AND L5
L10             2 S L7 OR L9

=> d l2
L2 HAS NO ANSWERS
L2                STR
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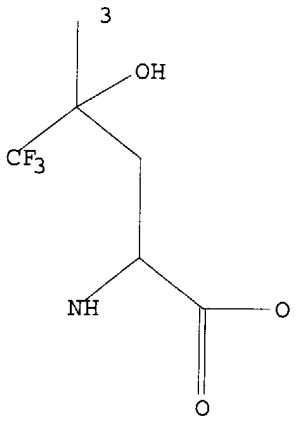


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Structure attributes must be viewed using STN Express query preparation.


=> d l2 d bib abs hitstr 1-2
L2 HAS NO ANSWERS
'D BIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data.  (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
          map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d l10 bib abs hitstr 1-2

L10  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:816776  CAPLUS
DN   138:39519
```

TI A Short and Efficient Synthesis of L-5,5,5,5',5',5'-hexafluoroleucine from N-Cbz-L-Serine

AU Anderson, James T.; Toogood, Peter L.; Marsh, E. Neil G.
CS Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA

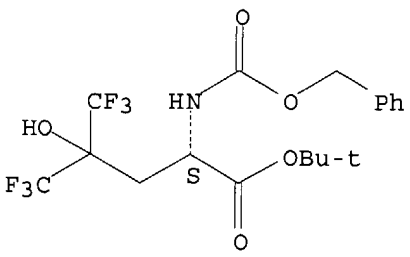
SO Organic Letters (2002), 4(24), 4281-4283
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 138:39519

AB 5,5,5,5',5',5'-Hexafluoroleucine, H2NCH(CO2H)CH2CH(CF3)2, a fluorous analog of leucine, is prepared from Cbz-L-Ser-OH by a short and efficient synthesis in 50% overall yield, 99% enantiomeric excess, and in multigram quantities. Key steps are addition of a serine-derived organozincate to hexafluoroacetone to construct the hexafluoroleucine side chain, followed by radical-mediated deoxygenation of the resulting tertiary alc.

IT **478548-20-8P 478548-21-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of hexafluoroleucine from Cbz-Ser with the addition of hexafluoroacetone to serine-zinc adduct followed by radical-mediated deoxygenation as key steps)

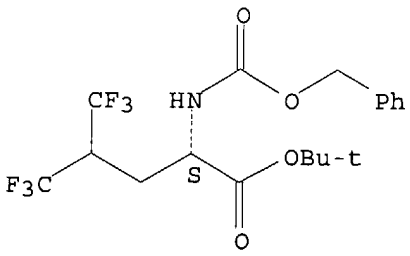
RN 478548-20-8 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-4-hydroxy-N-[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 478548-21-9 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

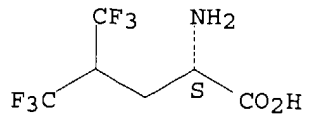
Absolute stereochemistry.



IT **149560-64-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of hexafluoroleucine from Cbz-Ser with the addition of hexafluoroacetone to serine-zinc adduct followed by radical-mediated deoxygenation as key steps)

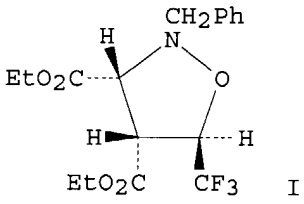
RN 149560-64-5 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

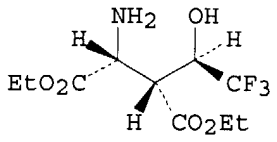


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:80452 CAPLUS
DN 118:80452
TI A cycloadditive route to trifluoromethyl-substituted amino alcohols
AU Bravo, Pierfrancesco; Bruche, Luca; Fronza, Giovanni; Zecchi, Gaetano
CS Cent. Stud. Sostanze Org. Nat., CNR, Milan, I-20133, Italy
SO Tetrahedron (1992), 48(44), 9775-88
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



I

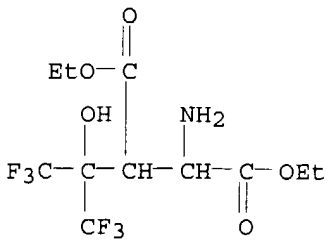


II

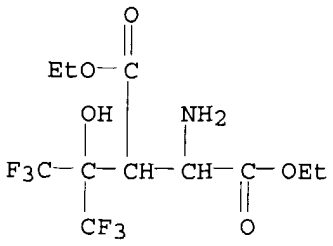
AB A synthetic approach to the title compds. is described, involving the 1,3-dipolar cycloaddn. of nitrones to trifluoromethyl-substituted alkene derivs. followed by reductive ring opening of the so obtained isoxazolidines. Thus, cycloaddn. of Et02CCH:N+(CH2Ph)O- to (F3C)CH:CHCO2Et gave isoxazolidine I which was hydrogenated to amino alc. II.

IT **145653-41-4P 145653-42-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

RN 145653-41-4 CAPLUS
CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, erythro- (9CI) (CA INDEX NAME)



RN 145653-42-5 CAPLUS
CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, threo- (9CI) (CA INDEX NAME)



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=> d his

     (FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

     FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004
L1             STRUCTURE UPLOADED
L2             STRUCTURE UPLOADED
L3            24 S L1 SSS FULL
L4             0 S L2 SSS
L5             3 S L2 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004
L6            11 S L3
L7             2 S L3 AND L5
L8             7 S L3/PREP
L9             2 S L8 AND L5
L10            2 S L7 OR L9

     FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004
L11            STRUCTURE UPLOADED
L12            0 S L11
L13            0 S L11

     FILE 'CAPLUS' ENTERED AT 11:20:56 ON 20 APR 2004

=> d l8 bib abs hitstr 1-7

L8   ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:816776  CAPLUS
DN   138:39519
TI   A Short and Efficient Synthesis of L-5,5,5,5',5',5'-hexafluoroleucine from
     N-Cbz-L-Serine
AU   Anderson, James T.; Toogood, Peter L.; Marsh, E. Neil G.
CS   Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA
SO   Organic Letters (2002), 4(24), 4281-4283
     CODEN: ORLEF7; ISSN: 1523-7060
PB   American Chemical Society
DT   Journal
LA   English
OS   CASREACT 138:39519
AB   5,5,5,5',5',5'-Hexafluoroleucine, H2NCH(CO2H)CH2CH(CF3)2, a fluorous
     analog of leucine, is prepared from Cbz-L-Ser-OH by a short and efficient
     synthesis in 50% overall yield, 99% enantiomeric excess, and in multigram
     quantities.  Key steps are addition of a serine-derived organozincate to
     hexafluoroacetone to construct the hexafluoroleucine side chain, followed
     by radical-mediated deoxygenation of the resulting tertiary alc.
IT   478548-20-8P 478548-21-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation of hexafluoroleucine from Cbz-Ser with the addition of
        hexafluoroacetone to serine-zinc adduct followed by radical-mediated
        deoxygenation as key steps)
RN   478548-20-8  CAPLUS
CN   L-Leucine, 5,5,5,5',5',5'-hexafluoro-4-hydroxy-N-[(phenylmethoxy)carbonyl]-
     , 1,1-dimethylethyl ester (9CI)  (CA INDEX NAME)

Absolute stereochemistry.
```
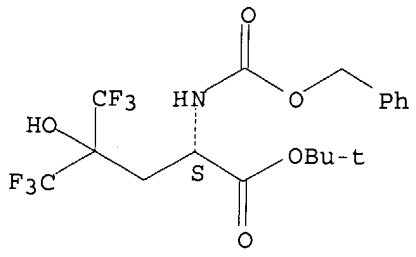
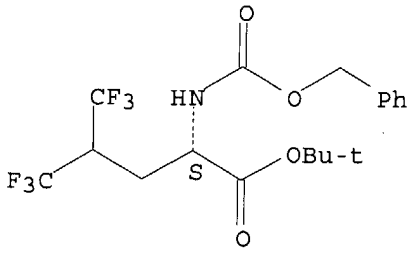



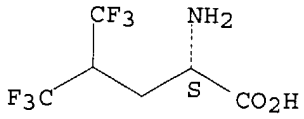
RN 478548-21-9 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **149560-64-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of hexafluoroleucine from Cbz-Ser with the addition of hexafluoroacetone to serine-zinc adduct followed by radical-mediated deoxygenation as key steps)
RN 149560-64-5 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:676148 CAPLUS
DN 137:201607
TI Synthesis of non-racemic hexafluoroleucine and its incorporation into peptides
IN Fichera, Alfio; Bilgicer, Zihni B.; Kumar, Krishna; Xing, Xuechao
PA Trustees of Tufts College, USA
SO PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002068592	A2	20020906	WO 2002-US5386	20020225
	WO 2002068592	A3	20030227		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-271999P P 20010227
US 2001-348091P P 20011029

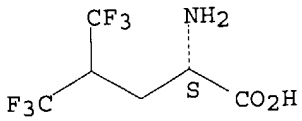
OS CASREACT 137:201607; MARPAT 137:201607

AB The invention relates to hexafluoroleucine and congeners for the synthesis of protein cores comprising hexafluoroleucine or congeners. Compds. R2NCH[CH2CH(CF3)2]CO-X-R1 [X = O, S, NR, CR2; R = H, alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, formyl, acyl, alkoxycarbonyl, aralkoxycarbonyl, alkylaminocarbonyl, or aralkylaminocarbonyl; R1 = H, alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; or XR1 = halide] are claimed. The stereochem. configuration at any stereocenter of these compds. may be R, S, (enantiomeric excess .gtorsim. 85%) or RS. A novel, short, and efficient synthesis of (S)-5,5,5,5',5',5'-hexafluoroleucine in > 99% ee was carried out starting from Garner's aldehyde, a protected oxazolidine aldehyde. Certain peptides comprising hexafluorleucine or congeners generally show higher thermal stability and enhanced resistance to chemical denaturation. Mixed hydrocarbon/fluorocarbon cores self-sort into homogeneous bundles, suggesting new avenues for the design and manipulation of protein-protein interfaces.

IT **201930-89-4P 340714-55-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of non-racemic hexafluoroleucine and its incorporation into peptides)

RN 201930-89-4 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX NAME)

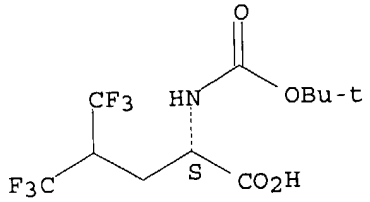
Absolute stereochemistry. Rotation (+).



● HCl

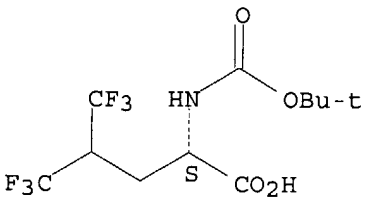
RN 340714-55-8 CAPLUS
CN L-Leucine, N-[(1,1-dimethylethoxy)carbonyl]-5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



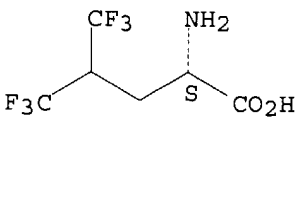
L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:234530 CAPLUS
DN 134:367168
TI A Novel Synthesis of Enantiomerically Pure 5,5,5,5',5',5'-Hexafluoroleucine
AU Xing, Xuechao; Fichera, Alfio; Kumar, Krishna
CS Department of Chemistry, Tufts University, Medford, MA, 02155, USA
SO Organic Letters (2001), 3(9), 1285-1286
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:367168
AB A novel, short, and efficient synthesis of (S)-5,5,5,5',5',5'-hexafluoroleucine (6) in greater than 99% ee was carried out starting from Garner's aldehyde, a protected oxazolidine aldehyde. The enantiomeric excess of the product was calculated from an NMR anal. of a dipeptide formed by reaction with a protected L-serine derivative Furthermore, a racemic sample of N-acylated hexafluoroleucine was enzymically resolved by treatment with porcine kidney acylase I and was found to have the same optical rotation as a synthetic sample of 6.
IT **340714-55-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of enantiomerically pure hexafluoroleucine)
RN 340714-55-8 CAPLUS
CN L-Leucine, N-[(1,1-dimethylethoxy)carbonyl]-5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **201930-89-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis of enantiomerically pure hexafluoroleucine)
RN 201930-89-4 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

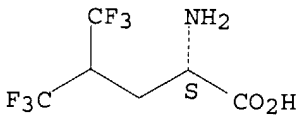


RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:79989 CAPLUS

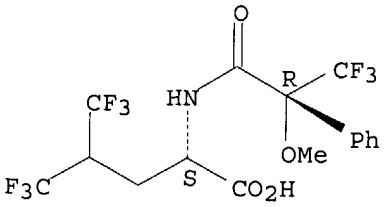
DN 128:128262
TI Asymmetric synthesis of (S)-5,5,5,5',5',5'-hexafluoroleucine
AU Zhang, Cong; Ludin, Christian; Eberle, Marcel K.; Stoeckli-Evans, Helen; Keese, Reinhart
CS Departement Chemie Biochemie, Universitaet Bern, Bern, CH-3012, Switz.
SO Helvetica Chimica Acta (1998), 81(1), 174-181
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta AG
DT Journal
LA English
AB (S)-(CF3)2CHCH2CHNH2CO2H is prepared starting from (CF3)2CO and bromopyruvate in 7 steps with 81% ee and 18% overall yield. Key step is the highly enantioselective reduction of the carbonyl group in (S)-(CF3)2CHCH2COCO2Et either by bakers' yeast (91% ee) or by catecholborane utilizing an oxazaborolidine catalyst yielding (R)-(CF3)2CHCH2CHOHCO2Et with 99% ee. The absolute configuration was determined by x-ray anal. of the HCl adduct of (2S)-N-[(R)-1-phenylethyl]-(S)-5,5,5,5',5',5'-hexafluoroleucine Et ester.
IT **149560-64-5P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(asym. synthesis and absolute configuration)
RN 149560-64-5 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



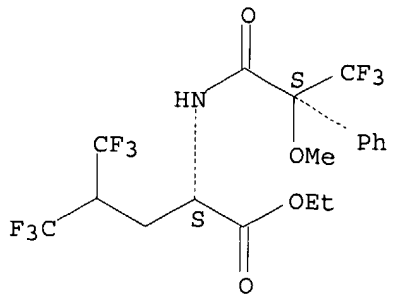
IT **201930-91-8P 201930-93-0P 201930-95-2P**
201930-97-4P 201930-98-5P 201930-99-6P
201931-01-3P 201931-02-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(asym. synthesis and absolute configuration)
RN 201930-91-8 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



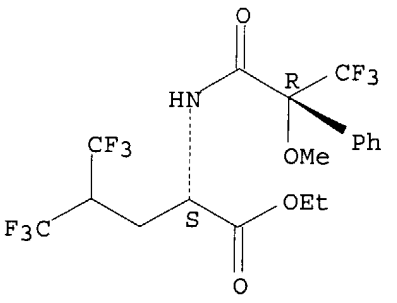
RN 201930-93-0 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



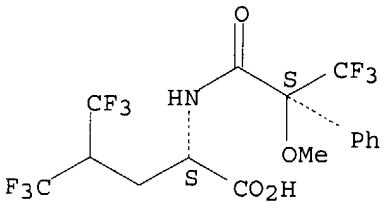
RN 201930-95-2 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



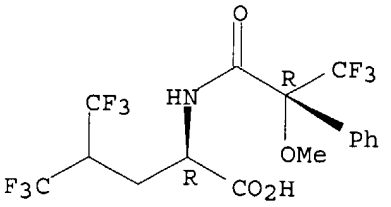
RN 201930-97-4 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 201930-98-5 CAPLUS
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

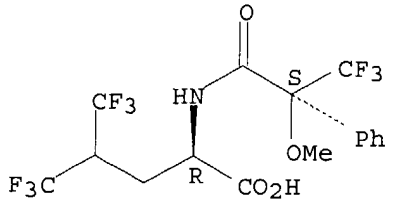
Absolute stereochemistry.



RN 201930-99-6 CAPLUS
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-

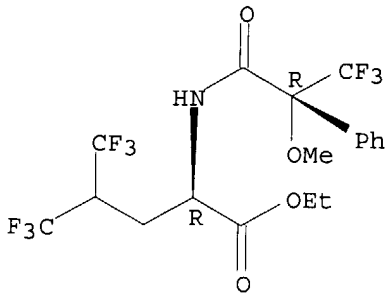
oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



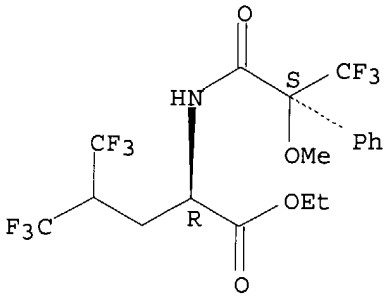
RN 201931-01-3 CAPLUS
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



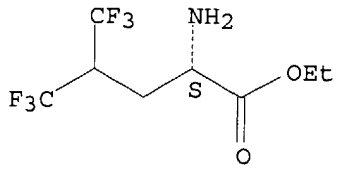
RN 201931-02-4 CAPLUS
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **201930-88-3P 201930-89-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(asym. synthesis of fluoroleucine)
RN 201930-88-3 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

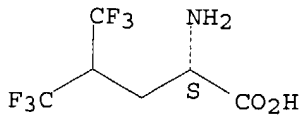
Absolute stereochemistry.



● HCl

RN 201930-89-4 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX NAME)

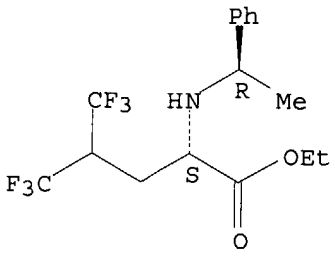
Absolute stereochemistry. Rotation (+).



● HCl

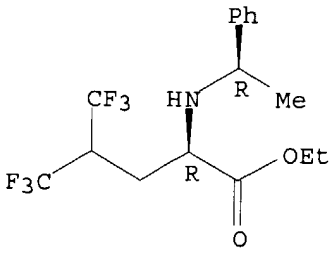
IT **201930-85-0P 201930-87-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(asym. synthesis of fluoroleucine)
RN 201930-85-0 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



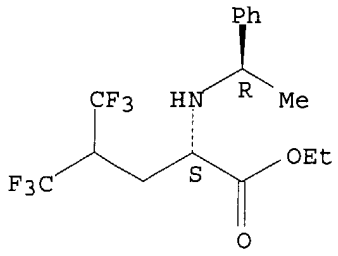
RN 201930-87-2 CAPLUS
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



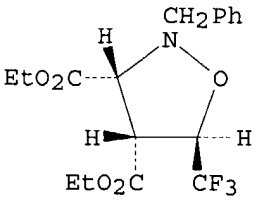
IT **201930-86-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(crystal structure; asym. synthesis of fluoroleucine)
RN 201930-86-1 CAPLUS
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

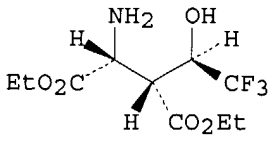


● HCl

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:80452 CAPLUS
DN 118:80452
TI A cycloadditive route to trifluoromethyl-substituted amino alcohols
AU Bravo, Pierfrancesco; Bruche, Luca; Fronza, Giovanni; Zecchi, Gaetano
CS Cent. Stud. Sostanze Org. Nat., CNR, Milan, I-20133, Italy
SO Tetrahedron (1992), 48(44), 9775-88
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI

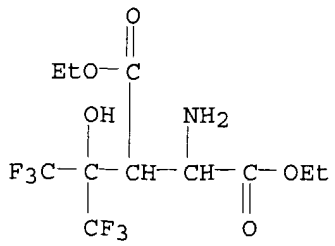


I

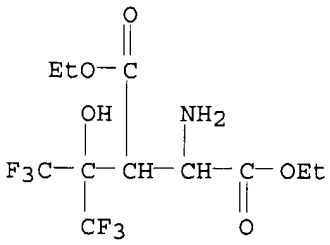


II

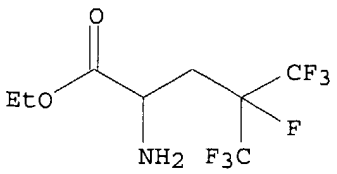
AB A synthetic approach to the title compds. is described, involving the 1,3-dipolar cycloaddn. of nitrones to trifluoromethyl-substituted alkene derivs. followed by reductive ring opening of the so obtained isoxazolidines. Thus, cycloaddn. of EtO2CCH:N+(CH2Ph)O- to (F3C)CH:CHCO2Et gave isoxazolidine I which was hydrogenated to amino alc. II.
IT **145653-41-4P 145653-42-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 145653-41-4 CAPLUS
CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, erythro- (9CI) (CA INDEX NAME)



RN 145653-42-5 CAPLUS
CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, threo- (9CI) (CA INDEX NAME)

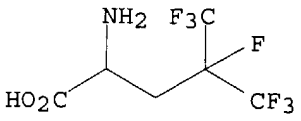


L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:468600 CAPLUS
DN 87:68600
TI Synthesis of fluorine-containing DL-alanine derivatives
AU Maki, Yasuo; Inukai, Kan
CS Ind. Res. Inst., Nagoya, Japan
SO Yuki Gosei Kagaku Kyokaishi (1976), 34(10), 722-5
CODEN: YGKKAE; ISSN: 0037-9980
DT Journal
LA Japanese
AB Preparation of DL-alanines having a perfluoroalkyl group at the β-position is described. Radical addition of CF3I, CF3CF2I, CF3(CF2)2I, and (CF3)2CFI to CH2:CHCO2Et under UV irradiation gave 23-34% α-iodo-β-(perfluoroalkyl)propionates (I). Reactions of I with NaN3 followed by catalytic hydrogenation gave 74-85% of the corresponding F-containing DL-alanine derivs. which on hydrolysis produced the free amino acids.
IT **63664-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 63664-53-9 CAPLUS
CN Norvaline, 4,5,5,5-tetrafluoro-4-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

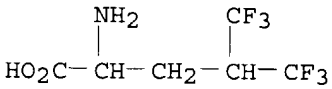


IT **63948-30-1P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

RN 63948-30-1 CAPLUS
CN Norvaline, 4,5,5,5-tetrafluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:78588 CAPLUS
DN 68:78588
TI Fluorinated analogs of leucine, methionine, and valine
AU Lazar, Joseph; Sheppard, William A.
CS Exptl. Sta., du Pont de Nemours, E. I., and Co., Wilmington, DE, USA
SO Journal of Medicinal Chemistry (1968), 11(1), 138-40
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB The fluorinated amino acid analogs trifluorovaline (I), hexafluorovaline (II), and trifluoromethionine (III) were prepared by known methods. Hexafluoroleucine, (CF3)2CHCH2CH(NH2)CO2H (IV), was prepared by treating (CF3)2CHCH2CO2H with LiAlH4, then with tosyl chloride in pyridine, giving a tosylate which was converted to (CF3)2CHCH2CH2CN by treatment with NaCN in Me2SO. This compound was hydrolyzed to the acid, treated with Br and SOCl2 to give the 2-bromo compound, esterified with EtOH, treated with NaN3 in EtOH, hydrogenated, hydrolyzed with HCl, and treated with pyridine to give the final product, IV. The pKa of these compds. and their amino acid analogs are given. In biol. studies, the growth of Escherichia coli B-14 Leu- was not supported by IV, and I, II, and III did not support the growth of valine and methionine auxotrophs of E. coli K12. The growth of wild type E. coli B and K12 was not inhibited by the F-containing compds., but the latter were not incorporated into the cell protein.
IT **16063-98-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 16063-98-2 CAPLUS
CN Valeric acid, 2-amino-5,5,5-trifluoro-4-(trifluoromethyl)- (8CI) (CA INDEX NAME)



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